A Strength Model for Materials with Phase Transformations

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A material model has been developed for the deviatoric components of the stress, which includes the effects of phase transformations. The model accounts for the different material properties of each phase and evolves separate yield surfaces. Relying on a free energy approach, the strength model is coupled to the equation of state, which is applicable to high-pressure applications. The material model has been implemented into a three-dimensional, Lagrangian, finite-element computer code. Results for a simulation demonstrate the importance of including phase transformations for an explosively loaded zirconium (Zr) plate.

Experimental results for the behavior of metals in the titanium group indicate that phase transformations can be an important mechanism in their response to deformation. For example, in Zr plate impact experiments, the phase change is apparent from the VISAR record of the back surface velocity [1]. Plate impact experiments represent a pressure dominated material response, which for purposes of matching the back surface velocity, may be accurately modeled without a sophisticated material strength model. For more general loadings, however, the effects of phase-change on the deviatoric response of the material are important. In order to improve computer simulations that involve solid-solid phase transformations, an isotropic strength model for multiple solid phases has been developed. The model allows each phase to have unique material properties such as the elastic moduli. It also includes a separately evolving yield stress for each phase.

For a material that undergoes a solid-solid phase change, the Helmholtz free energy (Ψ) for the mixture is written as a mass-weighted sum over the phases of the Helmholtz free energies of the individual phases [$\psi_k(\bar{\bar{\varepsilon}}_k^e, T_k)$, where $\bar{\bar{\varepsilon}}_k^e$ is the elastic strain tensor, T_k is the temperature of the kth phase] plus a term representing the mixing between the phases (Ψ^{mix}) [2–6]. For this development, we assume that the energy due to mixing is negligible ($\Psi^{mix} = 0$). The stress for a phase is decomposed into its volumetric and deviatoric components, which are related to the free energy

$$\bar{\bar{\sigma}}_k = \bar{\bar{s}}_k - P_k \bar{\bar{\delta}} = \frac{1}{v_k}\frac{\partial \psi_k}{\partial \bar{\bar{e}}_k^e} + \frac{\partial \psi_k}{\partial v_k}\bar{\bar{\delta}}. \quad (1)$$

In Eq. 1, $\bar{s}_k(\bar{e}_k^e, T_k)$ is the deviatoric stress, $P_k(v_k, T_k)$ is the pressure, v_k is the specific volume, $\bar{e}_k^e$ is the deviatoric elastic strain, and $\bar{\bar{\delta}}$ is the Kronecker delta. The free energy is assumed to be separable into its volumetric (Ψ_k^{eos}) and deviatoric (Ψ_k^{dev}) components. The volumetric component of the free energy provides the equation of state for the material under consideration. For Zr, this component of the free energy was determined by Greeff. It is written as the sum of static lattice energy, an ion motion free energy, and an electron excitation free energy contribution [7]. The deviatoric stress in each phase is related to the elastic part of the deviatoric strain of that phase

$$\bar{\bar{s}}_k = 2\mu_k \bar{\bar{e}}_k^e = 2\mu_k(\bar{\bar{e}}_k - \bar{\bar{e}}_k^p) \quad (2)$$

where $\bar{e}_k^p$ is the plastic strain of kth phase. It is assumed that all of the phases are in temperature and stress equilibrium (i.e., the Reuss limit). A mixture equation for the deviatoric components of the stress and strain may be obtained [8], which we present in incremental form

$$d\bar{s} = 2\mu \, d\bar{\bar{e}}^e = 2\mu(d\bar{\bar{e}} - d\bar{\bar{e}}^p). \quad (3)$$

In Eq. 3, the shear modulus (μ) and the strains ($d\bar{e}, d\bar{e}^e, and\ d\bar{e}^p$) are volume averaged quantities. It is observed that for this development the increment of the total strain ($d\bar{e}$) is split into the elastic ($d\bar{e}^e$) and inelastic or plastic ($d\bar{e}^p$) contributions. The increment of total

strain is obtained from the velocity gradients, which are computed from the global conservation of momentum.

To complete the formulation for the deviatoric component of stress, it is necessary to provide a constitutive equation for the plastic strain. Assuming associative flow plasticity, the plastic strain increment may be written as

$$d\varepsilon_k^p = d\overline{\overline{e}}_k^p = \frac{\partial f_k}{\partial \overline{\overline{s}}} d\lambda_k = 3\overline{\overline{s}}\, d\lambda_k; \qquad (4)$$

In Eq. 4, f_k is the yield function and $d\lambda_k$ is the plastic multiplier for the kth phase. For this development, separate von-Mises yield functions are used for each of the phases

$$f_k = \tau^2 - \sigma_k^2 . \qquad (5)$$

In Eq. 5, τ is the second invariant of the deviatoric stress or the von Mises stress, σ_k is the flow stress, and $f_k = 0$ represents the yield surface. The proposed model may utilize any general flow stress model, which includes, for example, the effects of strain and strain-rate hardening as well as thermal softening.

For the conditions of equilibrium, the existing phase is determined by the phase with the minimum Gibbs free energy ($G_k = \Psi_k + P\nu_k$). Singh [9] observed that the transformation rate is an exponential function of the pressure, which is reflected in the phenomenological model proposed by Greeff [1]
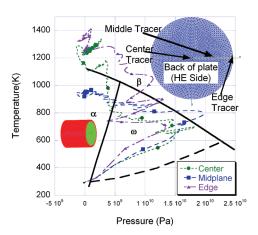
$$\dot{\xi}_j = (1 - \xi_j)\sum_{i \neq j} \nu_{ij} \frac{G_i - G_j}{B_{ij}} \exp\left(\frac{G_i - G_j}{B_{ij}}\right)^2 \quad (6)$$

where ν_{ij} and B_{ij} are constants that describe the rate at which the material transitions to phase j from phase i.

The model has been implemented into a Lagrangian finite element code [10] and verified through several simple loading cases. For complex deformations, the accurate modeling of the phase change in the material is important. For example, we simulate an explosively loaded plate. A cylindrical case is filled with high explosive and has a Zr plate on one end (see Fig. 1). The high explosive is set off using a point detonation along the axis of the cylinder at the opposite end from the Zr plate. The detonation punches the plate into a parabolic shell. Three material points on the underside of the plate are selected as tracer particles: one in the center, one at the middle radius, and one on the edge. At the tracer particles, the state variables are output as a function of time. The figure depicts the pressure-temperature phase diagram of Zr with the three tracer particles trajectories overlaid. All three particles translate in pressure-temperature space across all three of the phases of Zr. The center and edge particles end in the β phase as a final state, and the midradius particle ends in the α phase. Most of the material within the plate returns to the α phase, with the exception of the center and outer ring, which are in the β phase. A very small amount of material is in the ω phase for the final deformation (not shown).

Fig. 1.
Trajectories in pressure/temperature for three material points of an explosively loaded plate. Solid black lines are the boundaries between the phases and the black dashed line is the Hugoniot.

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[1] C.W. Greeff, et al., *AIP* **CP706**, 209–212, (2003).
[2] D.J.Andrews, *J. Comput. Phys.* **7**, 310 (1971).
[3] D.J. Andrews, *J. Phys. Chem. Solids* **34**, 825 (1973).
[4] J. Lemaitre and J.-L. Chaboche, *Mechanics of Solid Materials* (Cambridge University Press, New York, NY, 1985).
[5] J.G. Boyd and D.C. Lagoudas, *Int. J. Plast.* **12** (6), 805 (1996).
[6] D.A. Porter and K.E. Easterling, *Phase Transformations in Metals and Alloys* (Chapman and Hall, New York, NY, 1985).
[7] C.W. Greeff, submitted to *Modeling and Simulation in Materials Science and Engineering*, 2005.
[8] D.C. Wallace, *Thermodynamics of Crystals* (Dover Publications, Inc., Mineola, NY, 1972).
[9] A.K. Singh, et al., *J. Appl. Phys.* **53**, 1221 (1982).
[10] G.R. Johnson, et al., Wright Laboratory, Armament Directorate, Eglin Air Force Base report, WL-TR-1997-7037 (1997).